

STRUCTURE ACTIVITY TEAM REPORT ver. 04/98

Case #: L-08-0037

DCN:

SAT Date: 11/2/2007

SAT Chair:

~~11/02/2007~~

V. NAbholz

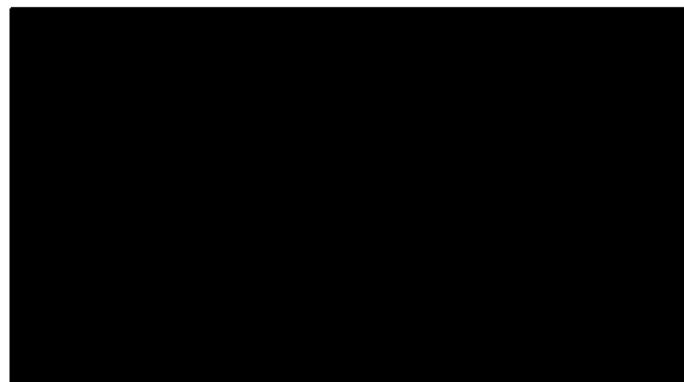
Submitter:

Chemical Name:

CAS RN:

Trade Name:

Structure



2007.11.23 11:11:04

Molecular Formula:

Molecular Wt.

WT%<500:

WT%<1000:

MP:

BP:

Eq. Wt:

H2O Sol (g/L):

Dispersible V.P.

<0.0325

Max. Prod. Volume (kg/yr):

Physical State:

Solid

USE:

Emulsifier for polymerization reactions.
There is 1 reference in file CA on STN.

Related Case Numbers

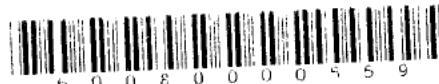
Case Role

Related Gas

Focus Date: NOV 19 2007

Results:

Page 1 of 9



STRUCTURE ACTIVITY TEAM REPORT 02 November 2007

CASE NUMBER: L08-0037

RELATED CASES:

CONCLUSIONS/DISCUSSIONS

TYPE OF CONCERN: HEALTH ECOTOX

LEVEL: 3 3

KEYWORDS: IRR-S, LIVER, REPRO, DEVEL, IMMUNO, ONCO, AQUATOX-A,C, LUNGS

SUMMARY OF ASSESSMENT:

FATE:

solid with mp = sublimes at 204 C (M)
log Kow = 2.0 (EPI)
S = dispersible (P)
vp < 0.032 mm Hg or torr at 25 °C (P)
bp = sublimes at 204 C (M)
H < 1.0E-8 (P)
log Koc = 3.1 (P)
log fish BCF = 0.50 (P)
sorption to sludge = moderate
submitted test data for aerobic biodegradation were:
22% biodegradation in 28 d via CO2 (Closed bottle [OECD301D]),
thus, not readily biodegradable
POTW removal = 0%
time for complete ultimate aerobic biodegradation > months
sorption to soils and sediments = moderate
PBT Potential: P2B1T3
*CEB FATE: migration to ground water = moderate

HEALTH: Absorption poor thru skin, good thru lungs, and moderate thru GI tract based on analogs;

submitted test data with this PMN were:
rat acute oral LD100 = 2.0 g/kg with systemic toxic signs, with
NOEL = 300 mg/kg;
moderate skin irritation in rabbits;
severe eye irritation in rabbits;
Ames test was negative;
E. coli test was negative;
no skin sensitization in mice up to 50% ai (LLNA);

[REDACTED]

4

H Ward95

530.0

1000.0

F
F

Predictions are based on SAR-test data for PFOA; SAR chemical class = PFOA; pH7; effective concentrations based on 100% active ingredients and mean measured concentrations; DW hardness < 150.0 mg/L as CaCO₃; and DW TOC < 2.0 mg/L; moderate concern for aquatic toxicity; high concern for reproductive toxicity to birds and wild mammals due to chronic toxicity observed in mammals; assessment factor = 10.0; concern concentration = 0.050 mg/L (ppm)
*CEB ECOTOX: All releases to the environment with CC = 50 ppb

SAT Co-chair: [REDACTED] [REDACTED]

10

GTOX Report

PMN No.

L-08-0037

CAS No.

[REDACTED]

Rcvd:

10/24/07

OECD

Incomplet

ID: Rec# 8 : 2

S/A
S

Name of Analog

[REDACTED]

Reviewer

[REDACTED]

with activation

without activation

Positive Strains

Salmonella Assay:

N

N

CHO:

[REDACTED]

[REDACTED]

Chromosomal Aberration

CHL:

[REDACTED]

[REDACTED]

V79:

[REDACTED]

[REDACTED]

E. coli Reverse Mutation:

N

N

Mouse Micronucleus Assay:

Route:

[REDACTED]

[REDACTED]

Rat Hepatocytes Unscheduled DNA Synthesis:

[REDACTED]

Other GTOX Results

A Salmonella assay was also provided for the analog

[REDACTED]

Comments

[REDACTED]

ECOTOX:

[REDACTED]

Fate:

Ready Biodegradability, (pg. 72-89)

WS/Log P:

WS => 87% w/w @ 20C (M, pg. 43), LogP = -0.403 (M, pg. 43).

Toxicology Report

PMN No.

L-08-0037

CAS No.

[REDACTED]

Rcvd:

10/24/2007

OECD

Incomplete

ID: Rec# 8 : 5

S/A

Name of Analog

S

[REDACTED]

Reviewer

[REDACTED]

Study#:

5

Study Type

EIRR

Species

RABB

Sex

NS

Route

EYES

Test Substance Description

white solid, purity: 96.4-100%, impurity: H substituted 3.6mol%

Test Conditions

Study duration: 240 minutes; Strain: NS; Wt/Life stage: NS; No. Groups/No. Per Group: 1/3; Controls: yes (2 eyes); Dose Level: 0.1 ml; Test Conditions (Dose regimen): The test material was applied onto the cornea of each of three enucleated eyes which had been maintained at a temperature of 32 C +/- 1.5 C within a superfusion chamber. Two control eyes were treated with saline solution. Measurements of corneal thickness were carried out pre-enucleation, post equilibration and up to 240 minutes following treatment.

Results

At the 60, 120, and 240 minute observations 23.4%, 28.5%, and 49.1% corneal swelling was observed, respectively. The test material was considered to have the potential to cause severe ocular irritancy in vivo.

Toxicology Report

PMN No.

L-08-0037

CAS No.

[REDACTED]

Rcvd:

10/24/2007

OECD

Incomplete

ID: Rec# 8 : 7

S/A

S

Name of Analog

[REDACTED]

Reviewer

EC

Study#:

7

Study Type

DSEN

Species

MICE

Sex

F

Route

DERM

Test Substance Description

white solid, purity: 96.4-100%, impurity: H substituted 3.6mol%, carrier: dimethyl formamide

Test Conditions

Study duration: 6 days; Strain: CBA/CaBkl; Wt/Life stage: 19-22 g/NS; No. Groups/No. Per Group: 3/4; Controls: positive control (a-Hexylcinnamaldehyde, Tech, 85%), 1/4; Dose Level: 25 ul; Test Conditions (Dose regimen): The study was conducted according to OECD 429 (skin sensitization: Local Lymph Node Assay). Following a preliminary screening, mice were exposed to 25 uL/ear of the test substance on the dorsal surface of the ear for 3 consecutive days. Five days following first application, mice were injected with 3H-methyl thymidine and then killed. Avicular lymph nodes were drained and pooled, and the stimulation indices were determined.

Results

Stimulation indices were 1.36, 1.27, and 2.68 following exposure to 10, 25, and 50% test substance, respectively. The test material was considered to be a non-sensitizer under the conditions of the test.

NCSAB SAT REPORT						Submitter					
PMN L-08-0037				CAS RN				Analog			
Chem.Name											
Structure										PV(kg)	
<div style="background-color: black; width: 100%; height: 150px;"></div>											
<div style="background-color: black; width: 100%; height: 30px;"></div>											
Formula						Eq Wt					
VW						Wt%<500				Wt%<1000	
MP (M)			MP (E) 204 (sublimes)			BP (M)			BP (E)		VP(E) <0.0325
NS g/L (E)			Dispersible WS g/L (M)			State			Solid		LogP(EPI)
Endpoint (mg/L)		Est. Value		Meas. Value		Comments				LogP(M)	
Fish 96-h										LogP(ClogP)	
Daphnid 48-h											
Algal 96-h											
Fish ChV											
Daphnid ChV											
Algal ChV											
ICF											
CHEMICAL CLASS:						SAR:					
COTOX CONCERN		H	M	L	CONCERN CONCENTRATION				HFOA		
IRSS DATE: 11/1/2007						ASSESSOR:					

ATTENDEES

SIGNATURE

CHEMISTRY

___ Paul Bickart
___ Diana Darling
___ Rich Engler
___ Greg Fritz
___ Daniel Lin
✓ Kathy Schechter

Kathy Schechter

ENVIRONMENTAL FATE

___ Bob Boethling
___ Wen-Hsiung Lee
___ Laurence Libelo
___ David Lynch
✓ Andy Mamantov

Andy Mamantov

HEALTH

✓ Katherine Anitole
✓ Michael Cimino
✓ Steve Cragg
✓ Leonard Keifer
___ David Lai
✓ Jim Murphy
___ Deborah Norris
___ Ronald Ward
✓ Yin Tak Woo

Katherine Anitole
Michael Cimino
Steve Cragg
Leonard Keifer
David Lai
Jim Murphy
Deborah Norris
Ronald Ward
Yin Tak Woo

ENVIRONMENTAL EFFECTS

___ Gordon Cash
___ Vince Nabholz
✓ Maggie Wilson

MEMO

SAT CHAIR/OTHER

___ Rebecca Jones
___ Leonard Keifer
✓ Vince Nabholz
___ Jim Kwiat

Vince Nabholz